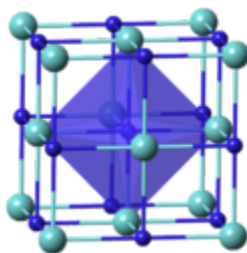


Tantalum carbide

Tantalum carbides (TaC) form a family of [binary](#) chemical compounds of [tantalum](#) and [carbon](#) with the empirical formula TaC_x, where *x* usually varies between 0.4 and 1. They are extremely [hard](#), brittle, [refractory ceramic](#) materials with metallic [electrical conductivity](#). They appear as brown-gray powders, which are usually processed by [sintering](#).

Tantalum carbide



Names

IUPAC name

Tantalum carbide

Other names

Tantalum(IV) carbide

Identifiers

CAS Number

(TaC): 12070-06-3 (https://commonchemistry.ca.s.org/detail?cas_rn=12070-06-3) ✓

(TaC_{0.5}): 12070-07-4 (https://commonchemistry.ca.s.org/detail?cas_rn=12070-07-4) ✗

3D model (JSmol)

(TaC): Interactive image (<https://chemapps.stolaf.edu/jmol/jmol.php?model=%5BTa%2B%5D%23%5BC-%5D>)

(TaC_{0.5}): Interactive image (<https://chemapps.stolaf.edu/jmol/jmol.php?model=%5BC%5D.%5BTa%5D.%5BTa%5D>)

ChemSpider

(TaC): 22369341 (<https://www.chemspider.com/Chemical-Structure.22369341.html>)

ECHA InfoCard

100.031.914 (<https://echa.europa.eu/substance-i>)

EC Number	information/-/substanceinfo/100.031.914) (TaC): 235-118-3 (TaC _{0.5}): 235-119-9
PubChem CID	(TaC): 159432 (https://pubchem.ncbi.nlm.nih.gov/compound/159432) (TaC _{0.5}): 166602 (https://pubchem.ncbi.nlm.nih.gov/compound/166602)
UNII	(TaC): 4ZUXHGUFHH (https://fdasis.nlm.nih.gov/srs/srsdirect.jsp?regno=4ZUXHGUFHH) ✓
CompTox Dashboard (EPA)	(TaC): DTXSID40893837 (https://comptox.epa.gov/dashboard/chemical/details/DTXSID40893837)
InChI (TaC): InChI=1S/C.Ta/q-1;+1 Key: DUMHRFXBHXIRTD-UHFFFAOYSA-N (TaC _{0.5}): InChI=1S/C.2Ta Key: VDBAWDHDCVOEAA-UHFFFAOYSA-N	
SMILES (TaC): [Ta+]#[C-] (TaC _{0.5}): [C].[Ta].[Ta]	
Properties	
Chemical formula	TaC
Molar mass	192.96 g/mol
Appearance	Brown-gray powder
Odor	Odorless
Density	14.3–14.65 g/cm ³ (TaC) 15.1 g/cm ³ (TaC _{0.5}) ^[1]
Melting point	3,768 °C (6,814 °F; 4,041 K) (TaC) ^[3]

	3,327 °C (6,021 °F; 3,600 K)
Boiling point	(4,780–5,470 °C (8,640–9,880 °F; 5,050–5,740 K) (TaC) ^{[1][2]}
Solubility in water	Insoluble
Solubility	Soluble in HF-HNO₃ mixture ^[1]
Thermal conductivity	21 W/m·K ^[2]
Thermochemistry	
Heat capacity (C)	36.71 J/mol·K ^[4]
Std molar entropy (<i>S</i> [⦿] ₂₉₈)	42.29 J/mol·K
Std enthalpy of formation (<i>Δ</i> _f <i>H</i> [⦿] ₂₉₈)	−144.1 kJ/mol
Related compounds	
Related refractory ceramic materials	Zirconium nitride Niobium carbide Zirconium carbide
<p>Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).</p> <p>✗ verify (https://en.wikipedia.org/w/index.php?title=Special:ComparePages&rev1=434321569&page2=Tantalum+carbide) (what is ✓✗?)</p> <p>Infobox references</p>	

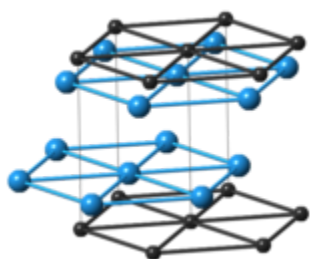
Being important [cermet](#) materials, tantalum carbides are commercially used in [tool bits](#) for cutting applications and are sometimes added to [tungsten carbide](#) alloys.^[5]

The melting points of tantalum carbides was previously estimated to be about 3880 °C depending on the purity and measurement conditions; this value is among the highest for binary compounds.^{[6][7]} And only [tantalum hafnium carbide](#) was estimated to have a higher melting point of 3942 °C.^[8] However new tests have conclusively proven that TaC actually has a melting point of 3768 °C and both [tantalum hafnium carbide](#) and [hafnium carbide](#) have higher melting points.^[9]

Preparation

TaC_x powders of desired composition are prepared by heating a mixture of tantalum and graphite powders in vacuum or inert-gas atmosphere ([argon](#)). The heating is performed at a temperature of about 2000 °C using a furnace or an arc-melting setup.^{[10][11]} An alternative technique is [reduction](#) of [tantalum pentoxide](#) by carbon in vacuum or hydrogen atmosphere at a temperature of 1500–1700 °C. This method was used to obtain tantalum carbide in 1876,^[12] but it lacks control over the stoichiometry of the product.^[7] Production of TaC directly from the elements has been reported through [self-propagating high-temperature synthesis](#).^[13]

Crystal structure



β -TaC_{0.5} with the unit cell, blue color is tantalum

TaC_x compounds have a [cubic](#) (rock-salt) crystal structure for $x = 0.7\text{--}1.0$,^[14] the lattice parameter increases with x .^[15] TaC_{0.5} has two major crystalline forms. The more stable one has an anti-[cadmium iodide](#)-type trigonal structure, which transforms upon heating to about 2000 °C into a hexagonal lattice with no long-range order for the carbon atoms.^[10]

Formula	Symmetry	Type	Pearson symbol	Space group	No	Z	ρ (g/cm ³)	a (nm)	c (nm)
TaC	Cubic	NaCl ^[15]	cF8	Fm $\bar{3}$ m	225	4	14.6	0.4427	
TaC _{0.75}	Trigonal ^[16]		hR24	R $\bar{3}$ m	166	12	15.01	0.3116	3
TaC _{0.5}	Trigonal ^[17]	anti-CdI ₂	hP3	P $\bar{3}$ m1	164	1	15.08	0.3103	0.4938
TaC _{0.5}	Hexagonal ^[11]		hP4	P6 ₃ /mmc	194	2	15.03	0.3105	0.4935

Here Z is the number of formula units per unit cell, ρ is the density calculated from lattice parameters.

Properties

The bonding between tantalum and carbon atoms in tantalum carbides is a complex mixture of ionic, metallic and covalent contributions, and because of the strong covalent component, these carbides are very hard and brittle materials. For example, TaC has a microhardness of 1600–2000 kg/mm²^[18] (~9 Mohs) and an [elastic modulus](#) of 285 GPa, whereas the corresponding values for tantalum are 110 kg/mm² and 186 GPa. The hardness, [yield stress](#) and [shear stress](#) increase with the carbon content in TaC_x.^[19]

Tantalum carbides have metallic electrical conductivity, both in terms of its magnitude and temperature dependence. TaC is a [superconductor](#) with a relatively high transition temperature of $T_C = 10.35$ K.^[15]

The magnetic properties of TaC_x change from [diamagnetic](#) for $x \leq 0.9$ to [paramagnetic](#) at larger x . An inverse behavior (para-diamagnetic transition with increasing x) is observed for HfC_x, despite that it has the same crystal structure as TaC_x.^[20]

Application

Tantalum carbide is widely used as sintering additive in [ultra-high-temperature ceramics](#) (UHTCs) or as a ceramic reinforcement in high-entropy alloys (HEAs) due to its excellent physical properties in melting point, hardness, elastic modulus, thermal conductivity, thermal shock resistance, and chemical stability, which makes it a desirable material for aircraft and rockets in aerospace industries.

Wang et al. have synthesized SiBCN ceramic matrix with TaC addition by mechanical alloying plus reactive hot-pressing sintering methods, in which BN, graphite and TaC powders were mixed with ball-milling and sintered at 1900 °C to obtain SiBCN-TaC composites. For the synthesis, the ball-milling process refined the TaC powders down to 5 nm without reacting with other components, allowing to form agglomerates that are composed of spherical clusters with a diameter of 100 nm-200 nm. TEM analysis showed that TaC is distributed either randomly in the form of nanoparticles with sizes of 10-20 nm within the matrix or distributed in BN with smaller size of 3-5 nm. As a result, the composite with 10 wt% addition of TaC improved the fracture toughness of the matrix, reaching 399.5MPa compared to 127.9MPa of pristine SiBCN

ceramics. This is mainly due to the mismatch of thermal expansion coefficients between TaC and SiBCN ceramic matrix. Since TaC has a larger coefficient of thermal expansion than that of SiBCN matrix, TaC particles endure tensile stress while the matrix endures tensile stress in radial direction and compressive stress in tangential direction. This makes the cracks to bypass the particles and absorb some energy to achieve toughening. In addition, the uniform distribution of TaC particles contributes to the yield stress explained by Hall-Petch relationship due to a decrease in grain size.^[21]

Wei et al. have synthesized novel refractory MoNbRe0.5W(TaC)_x HEA matrix using vacuum arc melting. XRD patterns showed that the resulting material is mainly composed of a single BCC crystal structure in the base alloy MoNbRe0.5W and a multi-component (MC) type carbide of (Nb, Ta, Mo, W)C to form a lamellar eutectic structure, with the amount of MC phase proportional to TaC addition. TEM analysis showed that the lamellar interface between BCC and MC phase presents a smooth and curvy morphology which exhibits good bonding with no lattice misfit dislocations. As a result, the grain size decreases with increasing TaC addition which improves the yield stress explained by Hall-Petch relationship. The formation of lamellar structure is because at elevated temperature, the decomposition reaction occurs in the MoNbRe0.5W(TaC)_x composites: $(\text{Mo, Nb, W, Ta})_2\text{C} \rightarrow (\text{Mo, Nb, W, Ta}) + (\text{Mo, Nb, W, Ta})\text{C}$ in which Re is dissolved in both components to nucleate BCC phase first and MC phase in the following, according to the phase diagrams.^[22] In addition, the MC phase also improves the strength of composites, due to its stiffer and more elastic property compared to BCC phase.^[23]

Wu et al. have also synthesized Ti(C, N)-based cermets with TaC addition with ball-milling and sintering at 1683K. TEM analysis showed that TaC helps dissolution of carbonitride phase and converts to TaC-binder phase. The resulting is a formation of “black-core-white rim” structure with decreasing grain size in the region of 3-5 wt% TaC addition and increasing transverse rupture strength (TRS). 0-3 wt% TaC region showed a decrease in the TRS because the TaC addition decreases the wettability between binder and carbonitride phase and creates pores. Further addition of TaC beyond 5 wt% also decreases TRS because TaC agglomerates during sintering and porosity again forms. The best TRS is found at 5wt% addition where fine grains and homogeneous microstructure are achieved for less grain boundary sliding.^[24]

Natural occurrence

Tantalcarbide is a natural form of tantalum carbide. It is a cubic, extremely rare mineral.^[25]

See also

- Tantalum hafnium carbide
- Hafnium carbide
- Hafnium carbonitride

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